Chapter

10

Optimization of Various Chemical and Biochemical Processes

10.1 Heat Exchanger Network Optimization

An important task during the design of chemical processes is to changing the process streams from their available temperatures to the required temperatures without additional cost. Heat recovery is an important approach for reducing the cost by using the heat available from streams to be cooled to the streams to be heated. The distinguish between hot streams and cold streams are made based on whether the stream is cooled or heated not on the basis of temperature. Developing an efficient energy system is very essential in process industry to reduce waste heat available. This waste heat from one process can be recovered and reused for another process. Heat Exchanger Network (HEN) is used to optimize this heat recovery consequently the investment cost and energy consumption in the process plant. Synthesis of HEN is one of the most commonly discussed problems in a process industry. This method has importance during determination of energy expenditure for a process and improving the recovery of energy in industry. The first systematic method was introduced in 1970s to heat recovery with the concept of pinch analysis. Hohmann (1971), and Linnhoff and Flower (1978) introduced the pinch analysis for synthesis of HEN. A single task is decomposed into three different subtasks (i.e., targets) like minimum utility cost, minimum number of units, and minimum investment cost network configurations. The major benefit of decomposing this HEN synthesis problem is that handling of these sub-problems are much simpler than the original single-task problem. The decomposed sub-problems are given below:

1. **Minimum utility cost** This subtask or target is related to the amount of maximum energy recovery that can be attained in a feasible HEN with a constant heat recovery approach temperature (HRAT), that allows to eliminate various non-energy efficient HEN structures. Hohmann in 1971, first introduced the minimum utility cost and then Linnhoff and Flower [Linnhoff and Flower, (1978)] discussed this technique. Cerda *et al.* (1983) discussed this as an LP transportation model and is improved as LP transshipment model by Papoulias and Grossmann [Papoulias and Grossmann (1983)].

2. **Minimum number of units** For a fixed utility cost, this target finds the match combination with the minimum number of units and distribution of their load. The overall cost of the HEN depends on the number of units. There are two popular models namely MILP transportation and MILP transshipment developed by various researchers (Cerda and Westerberg (1983), Papoulias and Grossmann (1983)). The vertical heat transfer formulation can also be employed to optimize HEN (Gundersen and Grossmann (1990) and Gundersen, Duvold and Hashemi-Ahmady (1996)).
3. **Minimum investment cost network configurations** This optimization is done based on the match information and heat load obtained from preceding targets. The NLP problem is formulated and optimization is done to minimize the overall cost of the network using the superstructure-based model developed by Floudas *et al.* [Floudas *et al.* (1986)]. In this model, the objective function is the investment cost of the heat exchangers (i.e., area of heat transfer only as matches and utility loads are fixed) that are proposed as a superstructure. The objective function is expressed as a function of temperatures, considering logarithmic mean temperature difference (LMTD) as driving temperature forces. This objective function is nonlinear and convex in nature. In addition, the constraints energy balance equations for the mixers and heat exchangers are nonlinear as they possess bilinear products of unknown flow rates times corresponding to unknown temperatures. The NLP problem formulation is nonconvex due to the bilinear energy balance equalities, which implies that use of local NLP solvers yield local solutions (Floudas and Ciric (1989)). Heat Exchanger Networks (HENs) synthesis is intrinsically a Mixed Integer and Nonlinear Programming (MINLP) problem. The theories of MINLP has been discussed in chapter 7 (section 7.2).

10.1.1 Superstructure

A simple HEN superstructure has been shown in Fig. 10.1. This superstructure comprised of four heat exchangers (HE1,HE2,HE3, and HE4) with two hot fluid and one cold fluid inlet.

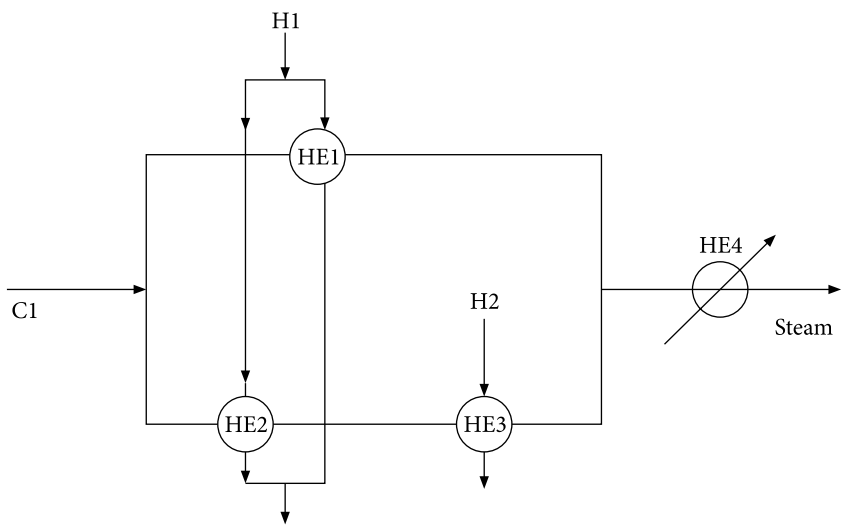

Fig. 10.1 HEN superstructure

10.1.2 Problem statement

The problem discussed in this section can be declared as follows, the condition given:

i. a set of hot process streams and a set of cold process streams for heat exchange with their specified flow rates, inlet and target temperatures, and physical properties (thermal conductivity, density, viscosity, heat capacity, and fouling factor)
ii. a single heating utility and a single cooling utility to fulfill the requirements of energy with their inlet and target temperatures as well as their physical properties
iii. capital and operating cost data involved in the network installation and operation.

During HEN design, determine the minimum overall annual cost target for these problems. We have to consider the target for the optimum power cost as well as traditional HEN design targets for minimum utilities, number of units and the heat transfer area.

The following assumptions were used in this work:

- The film heat-transfer coefficient of a stream is match independent.
- Considering the heat transfer in a single phase only.
- Only counter current and multi-pass shell-and-tube heat exchangers are considered.

The objective of HEN synthesis is to find out:

i. Optimal process flowsheet and design parameters.
ii. Values of temperatures and stream flow rates through the HEN and the process.
iii. Optimal configuration of the HEN including values for heat transfer area, number of units and requirement of utility.

10.1.3 Model formulation

Serna-González *et al.* [Serna-González *et al.* (2010)] have developed a HEN model, which considers both the fixed and operating costs.

The objective function is given by

$$\min TAC = A_f CC + C_U + C_P \tag{10.1}$$

where A_f is the annualized factor for investment, CC is the capital cost for heat exchange units, C_U is the hot and cold utilities costs, and C_P is the power cost.

The annual utility cost of a network is given by:

$$C_U = H_Y \left(C_H Q_{H_{\min}} + C_C Q_{C_{\min}} \right) \tag{10.2}$$

where $Q_{H_{\min}}, Q_{C_{\min}}$ are the minimum hot and cold utility target respectively.

C_H, C_C are unit cost of hot and cold utility respectively and H_Y represents the hour of operation of network per year.

Considering an equal distribution of area among all heat exchangers in the HEN, the network capital cost is given as

$$C_{CAP} = N_{u,mer}\left[a + b\left(A_{\min}/N_{u,mer}\right)^{c}\right] \tag{10.3}$$

where $N_{u,mer}$ is the minimum number of units for a maximum energy recovery network, $A_{\min}$ is the network area target, and *a,b* and *c* are cost law coefficients that depend on the type of heat exchanger, construction materials, and pressure rating.

In order to evaluate $A_{\min}$, we develop a mathematical model that is based on the spaghetti design model provided by the composite enthalpy-temperature curves. With a specified value of $\Delta T_{\min}$, for developing the spaghetti design of a process, the first step is to split the balanced composite curves into $k = 1,\ldots, K$ enthalpy intervals defined wherever a slope change occurs in either composite profile [Linnhoff and Ahmad (1990)]. The spaghetti design assumes that each hot stream i is integrated with all cold streams j within each enthalpy interval k. This generates a vertical structure for heat transfer, featuring parallel stream splitting and isothermal mixing. Under the assumptions that each stream match of the spaghetti design represents one and only one heat exchanger and that the film heat transfer coefficients of streams are match independent, the minimum area can be expressed as the sum of the stream contact areas:

$$A_{\min} = \sum_{i} A_{ci} = \sum_{j} A_{cj} \tag{10.4}$$

$$A_{ci} = \sum_{j=1}^{J}\left(\frac{1}{h_i} + \frac{1}{h_j}\right)\left(UA_{i,j}\right) \quad \text{for} \quad i \in I \tag{10.5}$$

$$A_{cj} = \sum_{i=1}^{I}\left(\frac{1}{h_i} + \frac{1}{h_j}\right)\left(UA_{i,j}\right) \quad \text{for} \quad j \in J \tag{10.6}$$

$$UA_{i,j} = \sum_{k=1}^{K} UA_{i,j,k} \quad \text{for} \quad i \in I, j \in J \tag{10.7}$$

$$UA_{i,j,k} = \frac{q_{i,j,k}}{F_{Tk}\Delta T_{MLk}} \quad \text{for} \quad i \in I, j \in J, k \in K \tag{10.8}$$

$$q_{i,j,k} = \frac{CP_{i,k}CP_{j,k}\Delta T_{i,k}}{\sum_{j} CP_{j,k}} \quad \text{for} \quad i \in I, j \in J, k \in K \tag{10.9}$$

where A_{ci} is the contract area of the hot stream i and A_{cj} is the contract area of the cold stream j. For each enthalpy interval k, $U_{i,j,k}$ is the UA value for the match between streams i and j, $q_{i,j,k}$ is the amount of heat transferred from hot stream i to cold stream j, $CP_{i,k}$ is the heat capacity flow rate of

hot stream i and $CP_{j,k}$ is the heat capacity flow rate of cold stream j. $\Delta T_{i,k}$ is the temperature change of any hot stream i, F_{Tk} is the correction factor for the log mean temperature difference, ΔT_{MLk} is the log mean temperature difference for any pair of streams.

If hot stream i is allocated in the shell side, the total stream pressure drop may be evaluated by the following equation [Linnhoff and Ahmad (1990)], [Serna-Gonzalez *et al.* (2004)].

$$\Delta P_i = K_i A_{ci} \left(\frac{1}{h_i} - R_{di} \right)^{-5.109} \quad \text{for} \quad i \in I \tag{10.10}$$

whereas if cold stream j is in the tube side,

$$\Delta P_j = K_j A_{cj} \left(\frac{D_{ti}}{D_t h_j} - R_{dj} \right)^{-3.5} \quad \text{for} \quad j \in J \tag{10.11}$$

where h_i and h_j are the dirt film heat transfer coefficient.

R_{di} is the fouling factor for hot stream i and R_{dj} is the fouling factor for hot stream j. Constants K_i and K_j depend on the stream physical properties and volumetric flow rate as well as the geometry of the heat exchanger.

The total cost of power, which is necessary for pumping the fluid streams, is given by:

$$C_P = \sum_i C_{P,i} Q_i \Delta P_i + \sum_j C_{P,j} Q_j \Delta P_j \tag{10.12}$$

where Q_i and Q_j are volumetric flow rate of the process streams i and j respectively. $C_{P,i}$ and $C_{P,j}$ are unit cost of power used by the streams i and j respectively.

For a given value of $\Delta T_{\min}$, Eqs (10.1)–(10.6) combined with Eqs (10.10)–(10.12) to develop a nonlinear programming (NLP) problem for minimization of the total annual cost of a HEN. The independent variables over which the minimization is carried out are the minimum network area, the stream contact areas, pressure drops of the streams and the film heat transfer coefficients. The values of the fixed parameters $q_{i,j,k}$, $UA_{i,j,k}$, and $UA_{i,j}$ have been calculated from Eqs (10.9), (10.8), and (10.7) respectively. Also, it should be noted that $Q_{H_{\min}}$, $Q_{C_{\min}}$, and $N_{u,mer}$ are calculated before the NLP problem is solved.

By varying the value of $\Delta T_{\min}$ used for utility targeting and recalculating the unit, area and power targets, the trade-off between capital and operating cost can be predicted to find the cost-optimal value of $\Delta T_{\min}$ for HEN design. The heat exchanger network synthesis (HENS) problem generally solved through sequential optimization [Floudas *et al.* (1986)] is incomplete, i.e., it is solved sub-optimally. In fact, minimizing the utilities consumption in the first step, then the number of matches required, and lastly the overall costs including the cost of the heat transfer area is definitely sub-optimal because the efficiency of each decision level depends on the quality of the solution found in the preceding decision level. In addition, the different economic issues involved are conjugated during the economic analysis of the energetic integration problem, which is not accomplished using the described series of partial sub-problems. The optimization problems developed for HEN synthesis are mostly MINLP. In mathematical programming methods, MINLP

problem can be solved by deterministic, stochastic or coupling of them. Deterministic methods like GBD, OA etc are sometimes failed to converge owing to mixed nature of binary and continuous variables. Stochastic methods such as Simulated Annealing (SA), and Genetic Algorithm (GA) can solve these problems efficiently.

10.2 Distillation System Optimization

Continuous distillation is one of the most widely used separation techniques in the chemical process industry. As large amount of energy is required, the optimum operation of continuous distillation columns has economic importance for process industries. During optimization of continuous distillation columns, for a specified degree of separation the problem of finding the optimal values of: (i) the number of stages, (ii) reflux ratio, (iii) feed location(s), have been addressed. In a typical distillation column, the choice of the operating parameters include fixing of the feed location and reflux ratio, whereas the number of stages becomes the design variable. The total (minimum) reflux condition, gives the minimum (infinite) number of stages [Ramanathan *et al.* (2001)].

The objective of such an optimization is the determination of the optimal operating and design parameters for achieving the desired degree of separation at the lowest total cost. The total cost of a distillation operation is made up of two major components. In the first component, the annual running cost of utilities i.e., the heating media to produce vapours, and the cooling media for vapour condensation, are accounted for. The second cost component refers to the annual fixed charges that take into account the interest and depreciation on the installation cost of the column, condenser, and reboiler; this component also includes maintenance of the installed equipment.

For optimizing the continuous distillation columns, the mixed integer non-linear programming (MINLP) seems to be an attractive approach [Viswanathan and Grossmann (1993)]. The MINLP formalism can be entrapped into a locally optimum solution instead of the desired globally optimum one. Moreover, MINLP methods are complex, computationally intensive and many simplifications become necessary to make them affordable [Wang *et al.* (1998)]. It is noticed, from the above discussion, that a majority of studies on continuous distillation optimization include applications of the deterministic optimization methods (MINLP, Powell's method, tunneling method, etc.). These formalisms are mostly calculus-based involving direct computation of the gradient. The gradient-based techniques invariably require the objective function to be smooth, continuous and differentiable (well-defined slope values). When the objective function is multimodal, noisy, and fraught with discontinuities, simultaneous fulfillment of these criteria cannot be guaranteed, thus, leading to suboptimal solutions. For instance, if the search space includes mixed integer (e.g., the number of distillation stages) and continuous (e.g., reflux ratio) variables, then the objective function could be non-monotonic and possess multiple local minima.

Continuous Simple Distillation

A simple continuous distillation column is given Fig. 10.2. This distillation column consists of feed (F), bottom product or residue (D), and distillate (D).

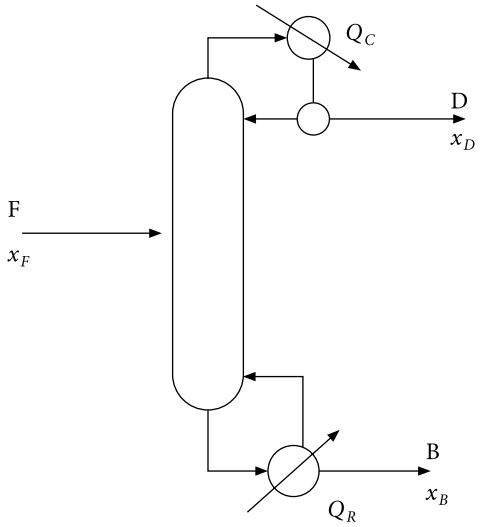

Fig. 10.2 Continuous distillation column

Problem Formulation

The objective function used in this study is representative of the total annual cost (C_T) that is made-up of two components, namely, the operating cost (C_1), and the fixed cost (C_2). While C_1 accounts for the energy cost pertaining to the reflux ratio and reboiler duty, the cost component C_2 accounts for the number of stages. The overall optimization objective is expressed as:

$$\text{Minimize } C_T(x) \quad x_k^L \le x_k \le x_k^U \tag{10.13}$$

where C_T is a function of the K-dimensional decision variable vector, $x = [x_1, x_2, \ldots x_k, \ldots x_K]^T$ and x_k^L and x_k^U respectively, refer to the lower and upper bounds on x_k. The three decision variables ($K = 3$) considered for optimization are: (i) the total number of stages (N), which is a function of real-valued x_1, (ii) reflux ratio (x_2), (iii) the feed location f_l (a function of x_3 and x_1). The evaluation procedure for the cost components C_1 and C_2 is discussed in Appendix I.

Computation of Total Cost

The objective function (C_T) for both, continuous simple and continuous azeotropic distillations represents the total annual cost ($). This cost comprises two additive components:

$$\text{Total Cost, } C_T = \text{ Energy Cost, } C_1 + (\text{depreciation} + \text{interest} + \text{maintenance}) \times (\text{Fixed Cost, } C_2) \tag{10.14}$$

where the energy cost, C_1, which is directly proportional to the heating cost is calculated according to:

$$C_1 = \frac{Q_R \times C_s \times N_D \times 24}{\lambda_{\text{steam}}} \tag{10.15}$$

where Q_R is the boiler duty; λ_{steam} is the latent heat of steam vaporization; C_s refers to the steam cost and N_D denotes the number of years working days.

The fixed cost, C_2 ($\$yr^{-1}$), consists of packing ($C_{\text{pack}}$) and column ($C_{\text{col}}$) cost where C_{pack} is computed as:

$$C_{\text{pack}} = A_c \times N \times HETP \times C^o_{\text{pack}} \tag{10.16}$$

Here, A_c representing the column area is calculated from the total vapor load on the basis of vapor velocity corresponding to the top temperature and capacity factor (C_f) of the packing (C_f = 1.5); C^o_{pack} denotes the packing cost per unit volume ($\$m^{-3}$) and the *HETP* value for the packing is in meter. The second cost component of C_2 i.e., C_{col}, is calculated on the basis of internals from the following correlation.

$$C_{\text{col}} = 3.14 \times 1.4 \times d_c \times N_{st} \times HETP \times W_s \times \rho_s \times C_{\text{steel}} \tag{10.17}$$

In this expression, d_c, W_s, ρ_s and C_{steel}, refer to the column diameter, column thickness (m), density (kgm^{-3}) of the column material (steel) and its cost ($\$kg^{-1}$). Assuming depreciation, interest, and maintenance costs of d (%), I (%) and m (%), respectively, the total annual cost to be minimized is evaluated as:

$$C_T = C_1 + (d + I + m)C_2 \tag{10.18}$$

In the operation of an azeotropic distillation column, a small quantity of entrainer is lost through the vent condenser and bottom product. Thus, the cost of entrainer loss approximately amounting to 3 per cent of the total entrainer quantity, must be additionally considered while evaluating C_T:

$$C_T = C_1 + (d + I + m)C_2 + C_3 \tag{10.19}$$

where, C_3 ($\$kg^{-1}$) refers to the cost of entrainer, i.e., benzene.

The solution to the minimization problem defined in Eq. (10.13) should satisfy the following constraints:

Purity constraints:

$$x_d^{\text{spec}} - x_d^{\text{simu}} \le 0 \tag{10.20a}$$

$$x_b^{\text{spec}} - x_b^{\text{simu}} \le 0 \tag{10.20b}$$

where x_d^{spec} and x_b^{spec}, represent the desired top and bottom concentrations (mole %) of the more volatile component, and x_d^{simu} and x_b^{simu} refer to the optimized (simulated) values of the top and bottom concentrations of the more volatile component.

Equality constraints:

As defined by the material balance, equilibrium, summation of the mole fraction and heat balance (MESH) equations.

Component material balance:

$$M_{ij} = \left(1 + \frac{S_i}{V_i}\right) \times v_{ij} + \left(1 + \frac{s_i}{L_i}\right) \times l_{ij} - f_{ij} - l_{i+1,j} - v_{i-1,j} \tag{10.21}$$

$$i = 2, \ldots, N-1;\ j = 1, 2, \ldots, C$$

Material balance for the reboiler and condencer:

$$M_{1j} = \left(1 + \frac{S_1}{V_1}\right) \times v_{1j} + \left(1 + \frac{s_1}{L_1}\right) \times l_{1j} - f_{1j} - l_{2,j} \tag{10.22}$$

$$M_{Nj} = \left(1 + \frac{S_N}{V_N}\right) \times v_{Nj} + \left(1 + \frac{s_N}{L_N}\right) \times l_{Nj} - f_{Nj} - v_{N-1,j} \tag{10.23}$$

where M_{ij} represents the discrepancy function expressed in terms of moles. hr^{-1}; S_i and s_i are the vapor and liquid side-streams, and f_{ij} refers to the feed flow.

Equilibrium relationship:

$$Q_{ij} = \frac{\eta_i \times m_{ij} \times V_i \times l_{ij}}{L_j} + \frac{(1 + \eta_i) \times v_{i-1,j} \times V_i}{V_{i-1}} - V_{ij} \tag{10.24}$$

where Q_{ij} represents the discrepancy function (moles.hr^{-1}); η_i is the Murphree stage efficiency, and m_{ij} represents the equilibrium constant for the component j on the ith stage. The UNIQUAC method was used to calculate m_{ij}.

Energy balance equation:

$$E_i = \left(1 + \frac{S_i}{V_i}\right) \times H_i + \left(1 + \frac{s_i}{L_i}\right) \times h_i - h_{fi} - H_{i-1} - h_{i+1} \tag{10.25}$$

$$i = 2, \ldots, N-1$$

Energy balance equations for the reboiler and condenser:

$$E_1 = \left(1 + \frac{S_1}{V_1}\right) \times H_1 + \left(1 + \frac{s_1}{L_1}\right) \times h_1 - h_{f1} - h_2 \tag{10.26}$$

$$E_N = \left(1 + \frac{S_N}{V_N}\right) \times H_N + \left(1 + \frac{s_N}{L_N}\right) \times h_N - h_{fN} - H_{N-1} \tag{10.27}$$

where E_i represents the discrepancy function (kcal.hr^{-1}); H_i and h_i are the enthalpy values for vapor and liquid respectively. To solve these equations a linear pressure and temperature profile was assumed. The pressure on the ith stage (p_i) is given by:

$$p_i = P_1 - i \times \Delta p \tag{10.28}$$

where P_1 is the bottom pressure and Δp refers to the pressure drop across the stage. The initial guess value for the temperature at each stage is given by:

$$T_i = T_1 + \frac{(i-1) \times (T_N - T_1)}{(N-1)} \tag{10.29}$$

where T_N and T_1 are the temperature of the condenser and reboiler respectively, that assume value of the boiling points of the more volatile component and less volatile component.

Napthali and Sandholm method [Napthali and Sandholm (1971)] has been utilized for the simulation of simple multi-component distillation to solve the steady-state MESH equations for each plate. The Napthali and Sandholm (NS) method uses the Newton–Raphson technique to simultaneously solve all the variables in the MESH equations. For simulation purposes, the full NS matrix method for the continuous distillation simulation is combined with the UNIQUAC method for predicting the vapour-liquid equilibrium (VLE).

10.3 Reactor Network Optimization

The reactor network is a very important part of many process industries. Efficient conversion of raw materials to desired products in the reactor division can greatly influence the process energy use, separation requirements consequently the overall economics. A reactor network contains different types of reactor with different streams (i.e., inlet, outlet, recycle). Economic feasibility of a chemical process strongly depends on the efficiency of the reaction system. Reactor network optimization aims to identify the most effective conceptual reactor design in terms of mixing and feeding strategies [Ashley and Linke, (2004)]. The objective of reactor network synthesis is to determine the types, sizes, and operating conditions of the reactor units in addition to the interconnections between the reactors, which convert the given raw materials into the desired products [Schweiger and Floudas (1999)]. The basis for the conceptual approach is to look closely at the fundamental relationships of the reaction process. For reactor networks, performance is generally defined by

objectives such as maximum yield, selectivity and conversion. These are all dependent on reaction rates that are based on component concentrations and temperature as described by the reaction kinetics.

The objective of reactor network synthesis is to determine the optimal mixing and feeding patterns that lead to the best possible performance attainable by a reactor network. The simplified models and representations are used to allow the quick identification of the optimal reactor network layout at a conceptual level. However, the optimization results need to be interpreted and translated into practical schemes by the engineer. Common features amongst optimal designs are serial arrangements of PFRs. This results from the discretization of PFRs by cascades of equal-volume CSTRs. Serial arrangements of PFRs allow for a finer discretization which leads to a better approximation of plug flow behaviour. Such structures should be interpreted by the design engineer as single PFRs.

Under the situation of known feed concentration and reaction kinetics, the job of reactor network synthesis (RNS) is to choose appropriate types of reactor, structures of the process and significant design parameters, which will optimize a particular objective function. Two important mathematical programming approaches for reactor networks synthesis are superstructure optimization and targeting [Jin *et al.* (2012)]

The superstructure based methods first introduce by Jackson in 1968 [Jackson, (1968)]. He considered a network composed of parallel plug flow reactors (PFRs) interconnected with side streams. Superstructure optimization involves generalized representations of ideal reactor units from which the optimal reactor mixing and feeding structure is to be extracted.

The superstructure representation consists of all possible combinations of reactor units. Reactor types are modelled as ideal CSTR, PFR and distributed side stream reactors (DSSR). Plug flow behaviour is approximated by a cascade of equal volume sub-CSTRs (Kokossis and Floudas, 1990). During optimization, it is ensured that there is always one reactor in existence, and that active reactors feature sequential connections with a minimum flow from the previous reactor. This maintains the expected sequential structure and allows optimization results to remain simple and interpretable.

Initially a network structure is recommended in superstructure optimization methods. Then from this initial network, an optimal sub-network that optimizes a preferred variable is obtained. The major advantages of superstructure optimization are that constraints can be included directly and conveniently, it is possible to modify the objective function and the optimal value of objective function and the reactor network can also be derived simultaneously. Although, the mathematical model of superstructure network is mostly a complicated non-linear programming problem (Schweiger and Floudas, 1999). This problem is very difficult to solve using the conventional optimization techniques. The topic is considered as an optimization problem where the objective function to be optimized is the yield or selectivity of a desired product, based on the complex reactions considered. The constraint problems are the material balances in the nodes of superstructure and the design equations of the reactors used. Kokossis and Floudas (1990) applied deterministic mixed integer nonlinear programming (MINLP) techniques to optimize superstructures comprising all possible combinations of continuous stirred tank reactors (CSTRs) and plug flow reactors (PFRs). More recently, stochastic techniques in the form of simulated annealing have been applied to the optimization of reactor network superstructures (Marcoulaki and Kokossis, 1996), with extensions to non-isothermal and multiphase systems by Mehta and Kokossis (2000).

Proposed superstructure

A simple superstructure is proposed [Silva *et al.* (2008)] to discuss the reactor network synthesis. Distinct possibilities of the typical CSTR-PFR arrangement have been considered. The most arrangement used in the literature are composed by a unique CSTR, a PFR solely, a CSTR followed by a PFR, a PFR followed by a CSTR or a CSTR and a PFR operating in parallel. Figure 10.3 shows us the proposed superstructure where all these combinations are available. The mathematical formulation is presented below.

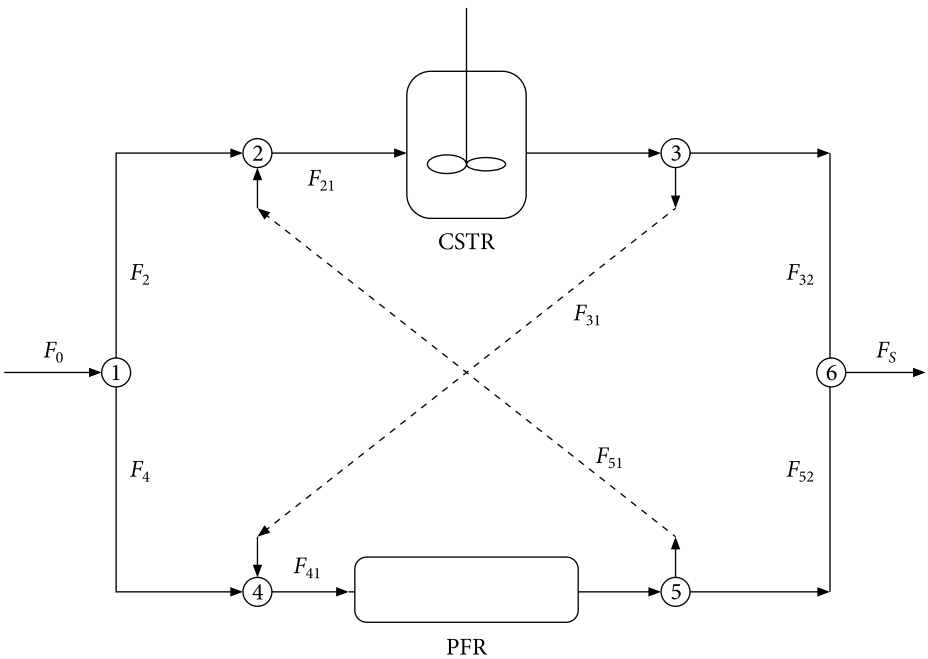

Fig. 10.3 Reactor network superstructure

Mathematical formulation

The formulation of mathematical model considers the mass balances in the nodes 1 to 6 of the superstructure. The feed introduced to the superstructure through the node 1. F_0 is the amount of initial feed, and it can be split randomly into two parts, F_2 and F_4. This can be written as:

$$F_2 = F_0 \times RAN1 \tag{10.30}$$

$$F_4 = F_0 - F_2 \tag{10.31}$$

Node 2 near the CSTR inlet is a mixing node. The inlet flow rate F_{21} is formed after the mixing the PFR outlet F_{51} and the branched flow rate F_2:

$$F_{21} = F_2 + F_{51} \tag{10.32}$$

Node 3 after the CSTR outlet is a splitting node. The CSTR outlet flow is F_3, which is equal to F_{21}, and can be split randomly into two parts, F_{31} and F_{32}:

$$F_{31} = F_3 \times RAN2 \tag{10.33}$$

$$F_{32} = F_3 - F_{31} \tag{10.34}$$

Again, node 4 near the PFR inlet is a mixing node. The inlet flow rate F_{41} is formed after the mixing of the CSTR outlet F_{31} and the branched flow rate F_4:

$$F_{41} = F_4 + F_{31} \tag{10.35}$$

And node 5 after the PFR outlet is a splitting node. The FPR outlet flow rate is F_5, which is equal to F_{41}, and can be split randomly into two parts, F_{51} and F_{52}:

$$F_{51} = F_5 \times RAN3 \tag{10.36}$$

$$F_{52} = F_5 - F_{51} \tag{10.37}$$

where random numbers $RAN1$, $RAN2$ and $RAN3$ are in between 0 and 1.

Node 6 is a splitting node and corresponds to the superstructure outlet. The outlet flow rate F_6 is represented by:

$$F_6 = F_{32} + F_{52} \tag{10.38}$$

These equations are the constraints for the superstructure. These constraints are used to formulate the optimization problem. The design equations developed for reactors used in this superstructure have to be considered as constraint equations. The design equation for the CSTR is:

$$\frac{V}{F} = \frac{x}{(-r)} \tag{10.39}$$

For the PFR, the design equation is:

$$F\frac{dx}{dV} = (-r) \tag{10.40}$$

where:

V = volume of reactor;

F = molar feed flow rate;

x = conversion;

$(-r)$ = rate of reaction.

The developed objective function depends on the reaction system used and it is solved to maximize yield and/or selectivity to a desired product. The superstructure equations and the algebraic and differential equations from the design of the reactors are used as constraints problem.

10.4 Parameter Estimation in Chemical Engineering

One of the fundamental tasks of engineering and science, and indeed of mankind in general, is the extraction of information from data. Parameter estimation is a subject that provides tools for the effective utilization of data in the evaluation of constants appearing in mathematical models and for assisting in modeling of phenomena [Beck and Arnold, (1977)]. The models may be in the form of algebraic, differential, or integral equations and their associated initial and boundary conditions.

Parameter estimation is a powerful tool for various engineering applications such as the design of process equipments. Actually, this technique offers the ability to estimate unknown parameters, which are often vital for the design and optimization. These methods use experimental data for determination of unknown parameters related to the model equations. During parameter estimation, we need to fit the experimental data with the model equation with minimum error. The name "parameter estimation" is not universally used. Other terms are non-linear least squares, non-linear estimation, non-linear regression.

10.4.1 Derivation of objective function

Mathematical models are normally utilized for many purposes such as analysis of experimental data, understanding the behavior of process, for process design, process optimization and process control. In most of the cases, we use the least square method for finding the best-fit model. The results found from the parameter estimation are somewhat uncertain because the data obtained from experiments are uncertain due to the presence of experimental errors. Characterization of this uncertainty is our primary concern for proper estimation of the ultimate results. Definition of the maximum likelihood function may be convenient to interpret the parameter estimation process [Schwaab *et al.* (2008)].

The experimental data is considered as random variables, whose joint probability distribution can be described by the following equation

$$P\left(z^{e}, z^{*}, V\right) \tag{10.41}$$

which expresses the probability to get the experimental values z^{e}, with the unknown real values z^{*} and a measure of the experimental errors V. The maximum likelihood estimation consist in maximizing Eq. (10.41), considering the model constraints

$$g\left(z^{*}, \theta\right) = 0 \tag{10.42}$$

where g is a vector of model functions and θ is a vector of model parameters. If we assume that the model is perfect and that the experiments have been performed properly, it is fair to acknowledge that the experimental outcomes are the most probable ones. Thus, efforts should be

made for maximizing the probability of getting these experimental results (Brad, 1974). While, the experimental errors follow the normal distribution, maximization of the likelihood function can be written as the minimization of the following function

$$S(\theta) = \left(z^* - z^e\right)^T V^{-1} \left(z^* - z^e\right) \tag{10.43}$$

where z is a vector that contains the independent x and dependent y variables and V is the covariance of measurements. When the objective function defined in Eq. (10.43) is used, the process is usually called data reconciliation. Considering that the independent variables x are known with high precision, then the objective function becomes

$$S(\theta) = \left(y^* - y^e\right)^T V_y^{-1} \left(y^* - y^e\right) \tag{10.44}$$

and we can rewrite the model equations as

$$y^* = f\left(x^*, \theta\right) \tag{10.45}$$

it is assumed that the dependent variables can be estimated (experimentally or numerically) as function of the model parameters and of the independent variables.

Whenever, the experimental measurements of the dependent variables are uncorrelated, the matrix Vy is diagonal and Eq. (10.44) takes the form of the known weighted least squares function

$$S(\theta) = \sum_{i=1}^{NE} \sum_{j=1}^{NY} \frac{\left(y_{ij}^* - y_{ij}^e\right)^2}{\sigma_{ij}^2} \tag{10.46}$$

where σ_{ij}^2 is the variance of the experimental fluctuations of the dependent variable j in the experiment i. The number of experiments and the number of dependent variables are represented by NE and NY respectively. When all variances are equal (this is generally assumed for models that have only one dependent variable), then Eq. (10.46) can be simplified to take the shape of the well-known least square function

$$S(\theta) = \sum_{i=1}^{NE} \left(y_i^* - y_i^e\right)^2 \tag{10.47}$$

The sum over different dependent variables was eliminated as the role of the least squares function is normally unsuitable for multi-response models. This is due to variations among the magnitudes of the responses and because of the involvement of various physical units. Matrix V provides the proper normalization and dimensionalization of each term in the sum.

After specifying the objective function, various numerical methods can be employed to minimize the objective function. The conventional derivative-based methods are used very frequently. These methods say that the minimization is done along a direction that combines gradient vector (vector of 1st derivatives with respect to model parameters) and the Hessian matrix (matrix of 2nd derivatives

with respect to model parameters) of the objective function. A class of methods called direct search methods (section 5.2) conduct the objective function minimization based on only the evaluation of the objective function, without the estimation of derivatives. Though, the concept of minimization without the computation of derivatives is very attractive, Bard [Bard (1974)] describes that gradient methods do better than direct search methods both in reliability and in speed of convergence. The direct and gradient search methods both are considered as local search methods as the search starts from an initial guess value and then results in a minimum. An excellent compilation of direct and derivative-based search processes has been discussed by Bard (1970, 1974).

For the application in chemical engineering field, minimization of the objective function in parameter estimation problems is very difficult and it may lead to severe numerical complication. These complexities arise due to many reasons such as large number of model parameters, a high correlation among the model parameters and multimodal nature of the objective function. The heuristic optimization methods such as SA, GA, and PSO (chapter 9) may be used to overcome these challenges. These algorithms are characterized by random search with the huge number of function evaluations. These techniques ensure a higher probability for finding the global minima, when compared to direct search and derivative-based search techniques. These algorithms do not need initial guess values for model parameters and do not utilize derivatives of the objective function.

These methods have been discussed in chapter 9. Pedro Mendes and Douglas B. Kell [Mendes and Kell (1998)] used to estimate the parameters for biochemical reaction. Their study shows that the Simulated Annealing and Levenberg-Marquardt methods (section 5.4) are most suitable for solving the optimization problem.

10.4.2 Parameter estimation of dynamic system

Problems on parameter estimation for nonlinear dynamic systems are described in this section [Moles *et al.* (2003)]. Here we have considered minimization of a cost function that determines the goodness of the fitted model with respect to a known experimental data set, subject to the system dynamics (as a set of differential equality constraints) in addition to other algebraic constraints. The mathematical representation of a nonlinear programming problem (NLP) with differential-algebraic constraints is as follows:

Find p to minimize

$$J = \int_0^{t_f} \left(y_{\text{msd}}(t) - y(p,t)\right)^T w(t) \left(y_{\text{msd}}(t) - y(p,t)\right) dt \tag{10.48a}$$

subject to

$$f\left(\frac{dx}{dt}, x, y, p, v, t\right) = 0 \tag{10.48b}$$

$$x(t_0) = x_0 \tag{10.48c}$$

$$h(x, y, p, v) = 0 \tag{10.48d}$$

$$g(x, y, p, v) = 0 \tag{10.48e}$$

$$p^L \le p \le p^U \tag{10.48f}$$

where J denotes the cost function to be minimized, p represents the vector of decision variables of the optimization problem; we have to estimate this set of parameters, y_{msd} is the experimental measure of a subset of the output state variables, $y(p, t)$ represents the predicted values for outputs from the model, $w(t)$ represents a matrix of scaling or weighting factors, x is the differential state variables, v denotes a vector of other parameters (usually time-invariant) that are not calculated, f is the set of algebraic and differential equality constraints explaining the dynamics of the system (i.e., the nonlinear process model), and h and g are the possible equality and inequality path and point constraints that represent additional requirements for the system performance. The vector p is subject to lower and upper bounds that can be considered as inequality constraints.

The formulated problem in Eq. (10.48) is a nonlinear programming problem (NLP) which has differential-algebraic (DAEs) constraints. Very often, these problems are multimodal (non-convex) due to the nonlinear and constrained nature of the system dynamics. Therefore, if these NLP-DAEs are solved using typical local optimization methods, for example the standard Levenberg–Marquardt method, it is obvious that the found solution will be of local nature, as explained by Mendes and Kell (1998). The simplest and earliest effort to overcome this non-convexity of many optimization problems have been developed based on the concept of repeatedly use of a local optimization algorithm, starting from a number of different starting point.

Example 10.1

A parameter estimation study has been given by Moles *et al.* [Moles *et al.* (2003)]. They estimated the parameters for biochemical pathways that consists of 36 kinetic parameters.

The mathematical formulation of this nonlinear dynamic model is:

$$\frac{dG_1}{dt} = \frac{V_1}{1 + \left(\frac{p}{Ki_1}\right)^{ni_1} + \left(\frac{Ka_1}{S}\right)^{na_1}} - k_1 G_1 \tag{10.49}$$

$$\frac{dG_2}{dt} = \frac{V_2}{1 + \left(\frac{p}{Ki_2}\right)^{ni_2} + \left(\frac{Ka_2}{M_1}\right)^{na_2}} - k_2 G_2 \tag{10.50}$$

$$\frac{dG_3}{dt} = \frac{V_3}{1 + \left(\frac{p}{Ki_3}\right)^{ni_3} + \left(\frac{Ka_3}{M_2}\right)^{na_3}} - k_3 G_3 \tag{10.51}$$

$$\frac{dE_1}{dt} = \frac{V_4 G_1}{K_4 + G_1} - k_4 E_1 \tag{10.52}$$

$$\frac{dE_2}{dt} = \frac{V_5 G_2}{K_5 + G_2} - k_5 E_2 \tag{10.53}$$

$$\frac{dE_3}{dt} = \frac{V_6 G_2}{K_6 + G_3} - k_6 E_3 \tag{10.54}$$

$$\frac{dM_1}{dt} = \frac{kcat_1 E_1 \left(\frac{1}{Km_1}\right)(S - M_1)}{1 + \frac{S}{Km_1} + \frac{M_1}{Km_2}} - \frac{kcat_2 E_2 \left(\frac{1}{Km_3}\right)(M_1 - M_2)}{1 + \frac{M_1}{Km_3} + \frac{M_2}{Km_4}} \tag{10.55}$$

$$\frac{dM_2}{dt} = \frac{kcat_2 E_2 \left(\frac{1}{Km_3}\right)(M_1 - M_2)}{1 + \frac{M_1}{Km_3} + \frac{M_2}{Km_4}} - \frac{kcat_3 E_3 \left(\frac{1}{Km_5}\right)(M_2 - P)}{1 + \frac{M_2}{Km_5} + \frac{P}{Km_6}} \tag{10.56}$$

where M_1, M_2, E_1, E_2, E_3, G_1, G_2 and G_3 represent the concentration of the component involved in the various biochemical reactions and S and P keep fixed initial values for each experiment (i.e., parameter under control). The remaining 36 parameters are considered to construct the optimization problem. These parameters are divided into two different categories: Hill coefficients, allowed to vary in the range (0.1,10) and all the others, allowed to vary in the range $(10^{-12},10^{+12})$.

The global optimization problem is represented as the minimization of a weighted distance measure, J, between predicted and experimental values of the 8 state variables, given as the vector y

$$J = \sum_{i=1}^{n}\sum_{j=1}^{m} w_{ij} \left\{ \left[y_{\text{pred}}(i) - y_{\text{exp}}(i) \right]_j \right\}^2 \tag{10.57}$$

where n and m are the number of data for each experiment and the number of experiments respectively, y_{exp} is the known experimental data, and y_{pred} represents the vector of states that corresponds to the predicted theoretical evolution using the model with a given set of 36 parameters. Additionally, w_{ij} represents the different weights considered to normalize the contributions of each term.

$$w_{ij} = \left(\frac{1}{\max\left[y_{\text{exp}}(i) \right]_j} \right)^2 \tag{10.58}$$

This problem (10.57–10.58) can be solved using nonlinear programming.

10.5 Environmental Application

In recent times, environmental pollution is the main issue for process industries. We need to reduce the quantity of effluent from industries and maintain the effluent standard as per environmental regulation. Optimization methods have been implemented successfully in the field of environmental pollution control. There are various ways by which environmental issues can be tackled. Upper limits of concentrations or pollutant flows in waste streams are set based on regulatory requirements. The designs that satisfy these constraints are evaluated in terms of economic indicators where we can include the cost of waste treatment and disposal in the economic objective function (Papalexandri and Pistikopoulos, 1996; Diwekar *et al.* 1992). The environmental issues can be implemented during process design of a chemical industry as constraints with the economic optimization, as objectives or as trading off the environmental objectives against other design objectives [García and Caballero (2012)]. Zhang *et al.* [Zhang *et al.* (2014)] have developed a multi-objective optimization method for municipal wastewater treatment. They simultaneously optimized the treatment cost and multiple effluent quality indexes (including effluent COD, $NH_4^+ - N$, $NO_3 - N$) of the municipal wastewater treatment plant (WWTP).

Air pollution control

Controlling the air pollution emissions is required to keep our environmental clean. There are various control methods that can be utilized to control air pollution emissions. Shaban *et al.* [Shaban *et al.* (1997)] formulated a mixed integer linear programming model that determines the best selection strategy. The objective of the program is to minimize the total control cost consisting of operating and investment costs. The development of the model has been discussed in following section. There are many constraints that are inflicted on the model including allocation constraints, time limits for utilization of each control process, maximum funds available for investment, and a pollution abatement level prescribed by regulatory body.

Model development

For developing the model, we are considering various emission sources; a number of pollutants are emitted from each source. There are many control options/technologies available for a given emission source. Updated and retrofit emission control devices in addition to improved operating procedures are among these pollution control technologies. A certain cost and reduction capacity is associated with each of these options. It is preferred to choose the best combination of control devices in an attempt to decrease emissions to a desired limit and, as a result, the total cost of the pollution control system is minimized. A mixed integer linear programming (MILP) model has been developed that will decide the optimal selection strategy. Different variables and parameters used to develop the model will be defined as:

Sets

I_i set of control options, which can be utilized on source i

J_i set of pollutants discharged from source i

K_j set of sources on which control j can be employed

Variables

T_j set-up time of control j (at which time the control device j is being made available).

T_{ij} time-length for which control j is utilized on source i.

x_{ij} binary variable that indicates whether control process j is used on source i ($x_{ij} = 1$) or not ($x_{ij} = 0$).

Parameters

C_j^0 installation or set-up cost of control device j.

$C_j^{\max}$ maximum set-up cost of control j (cost when control j is made available by its earliest possible availability time).

C_{ij} operating cost per unit time when control j is being used on source i.

B budget available for development of the control processes.

T_i start-up time for pollution source i.

$T_j^{\min}$ earliest time control j can be made accessible.

$T_j^{\max}$ latest time control j can be made accessible.

T length of time horizon of interest.

R_{ikj} total reduction per year of pollutant k in source i when control j is employed on source i.

K desired overall reduction of pollutant k.

P total number of pollutants from the various sources

Here, i represents the pollution source, j denotes the pollution control device, and k represents single pollutant.

Formulation of objective function

For each pollution source i, it is required to choose one control j in such a way that the total pollution cost will be minimized. The total cost is composed of the initial investment cost and the operating cost. The operating cost of all control processes over all pollution sources is represented by the following equation:

$$\text{Operating cost} = \sum_j \sum_{i \in K_j} C_{ij} T_{ij} \tag{10.59}$$

The investment cost is divided into two parts. A minimum fixed cost due to installation or set-up and an acceleration cost that is incurred when the set-up cost of a given control is speeded up. The set-up cost is given by:

$$\text{Set-up cost} = \sum_j C_j^0 \left(\sum_{i \in K_j} x_{ij} \right) \tag{10.60}$$

Whenever a control device j is not utilized on any of the pollution sources i, then in Eq. (10.60)

$$\sum_{i \in K_j} x_{ij} = 0 \tag{10.61}$$

Subsequently, the set-up cost associated with control j is reduced to zero as it should be.

The accelerated cost of a control j depends on how fast the set-up of the control is. For example, this cost is equal to its maximum $C_j^{\max}$ when the set-up time of control j is equal to its earliest possible set-up time $T_j^{\min}$. Also, the acceleration cost attains a minimum when the set-up time of control j is at its latest.

If we consider a linear relationship between set-up time and acceleration cost, then it can be expressed as:

$$\text{Acceleration cost} = aT_j + b \tag{10.62}$$

where

$$a = -\frac{C_j^{\max} - C_j^{\min}}{T_j^{\max} - T_j^{\min}} \tag{10.63}$$

$$b = -\frac{T_j^{\max} C_j^{\max} - T_j^{\min} C_j^{\min}}{T_j^{\max} - T_j^{\min}} \tag{10.64}$$

The decision variable T_j is as given before, the set-up time or time at which control j is being made accessible.

In order to make sure that the acceleration cost is always zero in the situation when control device j is not in use, Eq. (10.62) is modified as:

$$\text{Acceleration cost} = aT_j + b\sum_{i\in K_j} x_{ij} \tag{10.65}$$

If control device j is not selected, the 2nd term in the Eq. (10.65) is equal to zero

$$\left(\sum_{i\in K_j} x_{ij} = 0\right) \tag{10.66}$$

In such a case, the 1st term to be equal to zero, a condition should be imposed on the availability time T_j. This condition will be dealt with as constraints as discussed below. The objective function becomes

$$\min \sum_j \left\{ \left(aT_j + b\sum_{i\in K_j} x_{ij} + C_j^0 \sum_{i\in K_j} x_{ij} \right) + \sum_{i\in K_j} C_{ij} T_{ij} \right\} \tag{10.67}$$

Constraints

i. For each control device j to be considered for use on a source i; T_i, the start-up time of source i must be greater than $T_j^{\min}$, the earliest availability time of control j:

$$x_{ij}\left(T_j^{\min} - T_i\right) \le 0 \quad \forall j, i \in K_j \tag{10.68}$$

ii. For each source i, at most one control j can be used:

$$\sum_{j \in I_i} x_{ij} \leq 1 \quad \forall i \tag{10.69}$$

iii. Each control process j can be used at most once:

$$\sum_{i \in K_j} x_{ij} \leq 1 \quad \forall j \tag{10.70}$$

iv. Whenever, a control process j is not used for any of the pollution sources, then, the time T_j at which control j is being made available must be set to zero with the intention that control j will not have any effect on the overall cost. We can write this in equation form:

$$M \sum_{i \in K_j} x_{ij} \geq T_j \quad \forall j \tag{10.71}$$

where the parameter M signifies a large positive number. M should be set to the upper bound on T_j (i.e., $T_j^{\max}$) in order to have a tight constraint set. As given above, whenever control j is not utilized on any of the sources $i \in K_j$, then constraints in Eq. (10.71) ensure that $T_j = 0$. However, if control j is used on any of the sources i, then the constraint is rendered redundant and is always satisfied due to the presence of the large number M.

v. When a control process j is selected to utilize on source i (i.e., $x_{ij} = 1$), then the availability time of control j should be larger than the start-up time for source i (i.e., $T_j \geq T_i$). This can be given as the following equation:

$$T_j - x_{ix} T_i \geq 0 \quad \forall j, i \in K_j \tag{10.72}$$

vi. For each control process j, the availability time T_j is bounded between a minimum time $T_j^{\min}$ and a maximum time $T_j^{\max}$(i.e., $T_j^{\min} \leq T_j \leq T_j^{\max}$). However, the lower and upper bounds on j should be relaxed to zero when the control process j is not selected for use. This can be accomplished by the following:

$$\left(\sum_{i \in K_j} x_{ij} \right) T_j^{\min} \leq T_j \leq \left(\sum_{i \in K_j} x_{ij} \right) T_j^{\max} \quad \forall j \tag{10.73}$$

vii. When control j is used on source i, then $T_j \geq T_i$ and the time increment that j is used on i is $T_{ij} = T - T_j$. If j is not used on i, then $T_{ij} = 0$. The time period for use by each control process j on pollution source i is given below:

$$T_{ij} = \left(T - T_j \right) x_{ij} \quad \forall j, i \in K_j \tag{10.74}$$

The above set of constraints is nonlinear. Since, linear model equations are much easier to solve than nonlinear models, it is always advantageous to rearrange nonlinear constraints in the form of linear equations if it is possible [Glover, (1975); Ashford and Daniel, (1992)]. The method described by Raman and Grossman (1991) is used to rearrange the constraint given by Eq. (10.74) into linear form. For this reason, x_{ij} is associated with $T_{ij} \geq 0$ and $(1 - x_{ij})$ with $T_{ij} \leq 0$ and the constraint set is rewritten as:

$$L_1\left(1 - x_{ij}\right) \leq T_{ij} - T + T_j \leq U_1\left(1 - x_{ij}\right) \tag{10.75}$$

and

$$L_2 x_{ij} \leq T_{ij} \leq U_2 x_{ij} \qquad \forall j, i \in K_j \tag{10.76}$$

where L_1 = lower bound on $T_{ij} - T + T_j$, U_1 = upper bound on $T_{ij} - T + T_j$, L_2 = lower bound on T_{ij}, and U_2 = upper bound on T_{ij}.

Note that in the case when $x_{ij} = 1$, constraints 10.75, 10.76 reduce to:

$$0 \leq T_{ij} - T + T_j \leq 0 \tag{10.77}$$

and

$$L_2 \leq T_{ij} \leq U_2 \tag{10.78}$$

or simply $T_{ij} - T - T_j$, which is the desired result.

If, however, $x_{ij} = 0$, then constraints 10.75, 10.76 are rendered redundant due to proper use of the lower and upper bounds L_1, L_2, U_1, and U_2. Suitable choices for these bounds are discussed in Shaban *et al.* (1997).

viii. There is a certain budget B for process development; the investment to develop the control processes should not exceed the budget:

$$\sum_j \left\{ \left(aT_j + b \sum_{i \in K_j} x_{ij} \right) + C_j^0 \sum_{i \in K_j} x_{ij} \right\} \leq B \tag{10.79}$$

ix. It is required to reduce a given pollutant released to a designated reduction level:

$$\sum_j \sum_{i \in K_j} R_{ijk} T_{ij} \geq K \qquad \forall k = 1, 2, \ldots, P \tag{10.80}$$

x. Non-negativity and integrality:

$$T_{ij} \geq 0 \qquad \forall j, i \in K_j \tag{10.81a}$$

$$T_j \geq 0 \qquad \forall j \tag{10.81b}$$

$$x_{ij} = 0 \text{ or } 1 \quad \forall j, i \in K_j \tag{10.81c}$$

This problem is a MILP which can be solved by Branch and Bound method discussed in chapter 6.

Summary

- This chapter explains different optimization methods applied to the chemical and biochemical engineering. Heat exchanger network (HEN) and reactor network (RN) are the integrated part of any chemical process. HEN and RN have been optimized to get maximum profit. Distillation system is also optimized in this chapter. An optimized multi-component distillation system has been developed, which can be used in process industry. Parameter estimation is a very familiar technique to find the correlation between theoretical model and experimental data. Optimization methods can be used to find the best-fit model for a process. Beside these economic considerations, environmental pollution is required to consider during process development. We can incorporate this environmental issue with the design equation during its implementation.

Review Questions

10.1 What are the important factors we need to consider during heat exchanger network design?

10.2 Develop an optimization problem, which minimizes the operating cost a heat exchanger.

10.3 Draw the HEN superstructure with four heat exchangers.

10.4 Develop the model equation for a continuous distillation column with two feed inlet. How do you select the feed inlet position?

10.5 Discuss the algorithm of Napthali and Sandholm for solving MESH equations.

10.6 Develop a reactor network superstructure as shown in Fig. 10.3, considering both CSTR with volume V_1 and V_2.

10.7 Data is given below; use least square method to find the linear model.

x	3	5	7	9	10	15	20	22	25
y	12	18	22	32	38	53	67	72	78

10.8 Develop a model for wastewater treatment plant using MOO methods.

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